1/11

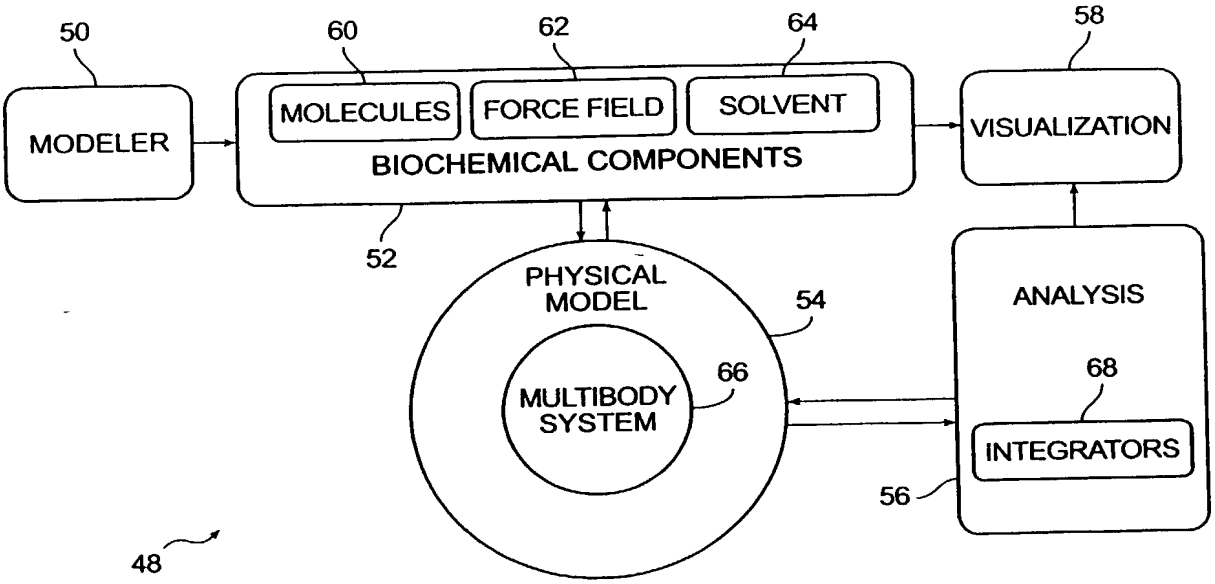
50
MODELER
60
62
64
MOLECULES
FORCE FIELD
SOLVENT
BIOCHEMICAL COMPONENTS
52
58
VISUALIZATION
PHYSICAL MODEL
54
MULTIBODY SYSTEM
66
ANALYSIS
68
INTEGRATORS
56
48

FIG. 1

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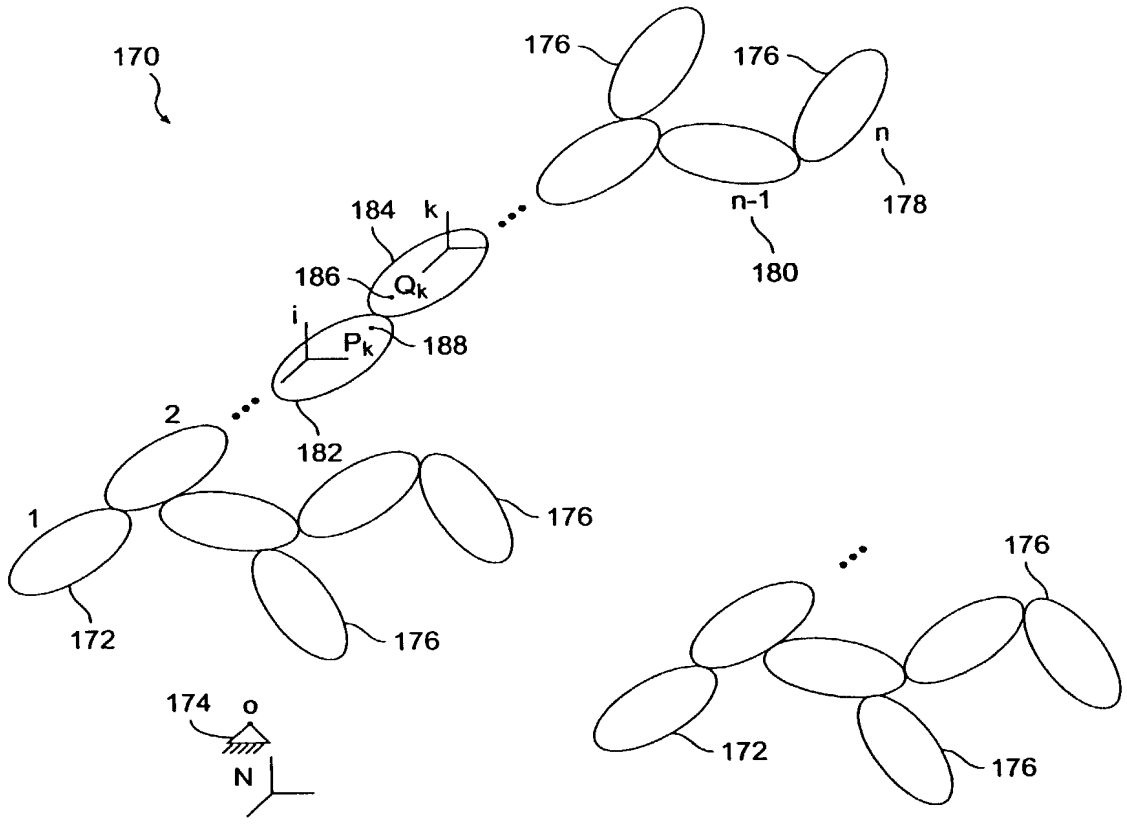
170
176
176
n
178
n-1
180
184
k
186
Q_k
i
P_k
188
182
2
1
172
176
176
176
172
176
174
o
N

FIG. 2

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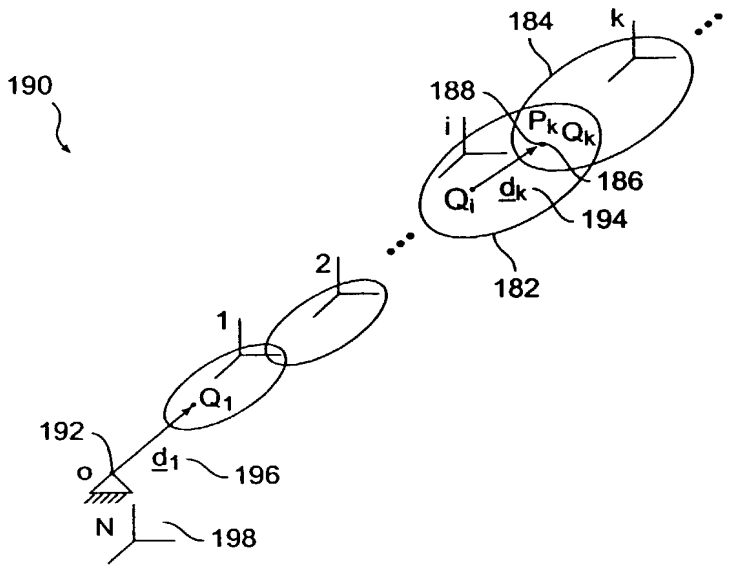
190
184
k
188
i
P_k Q_k
186
Q_i
$\underline{d}_k$
194
182
2
1
Q_1
192
o
$\underline{d}_1$
196
N
198

FIG. 3

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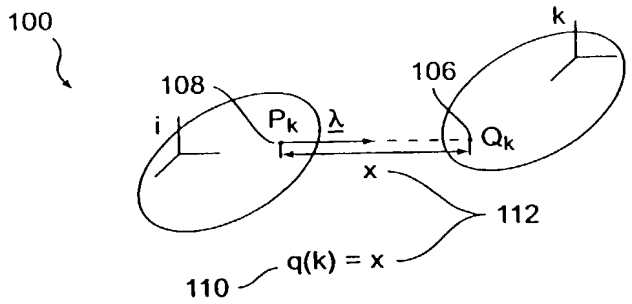

FIG. 4A

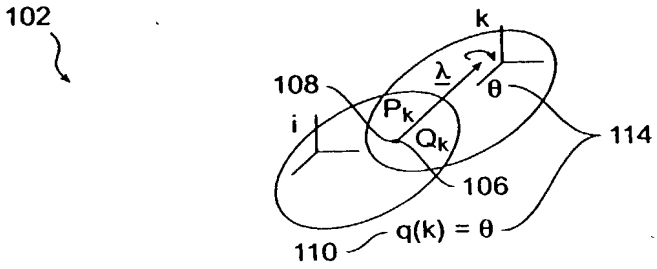

FIG. 4B

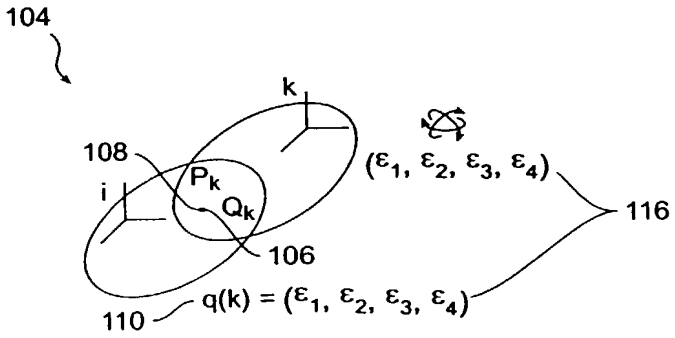

FIG. 4C

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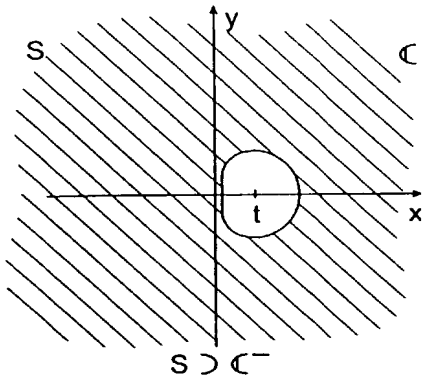
IMPLICIT EULER

$$R(z) = \frac{1}{1 - z}$$



$\lim_{z \to \infty} R(z) = 0$

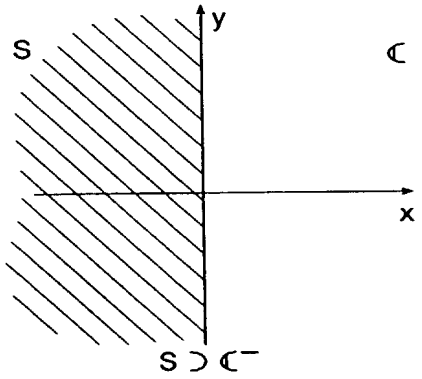
L–STABLE

A–STABLE

FIG. 5A

IMPLICIT MIDPOINT

$$R(z) = \frac{1 + z/2}{1 - z/2}$$



$\lim_{z \to \infty} R(z) \neq 0$

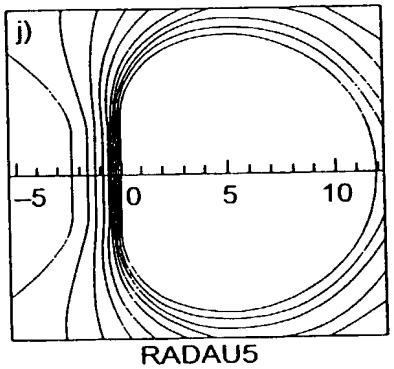
NOT L–STABLE

A–STABLE

FIG. 5B

RADAU5

$$R(z) = \frac{1 + 2z/5 + z^2/20}{1 - 3z/5 + 3z^2/20 - z^3/60}$$



$\lim_{z \to \infty} R(z) = 0$

L–STABLE

RADAU5

FIG. 5C

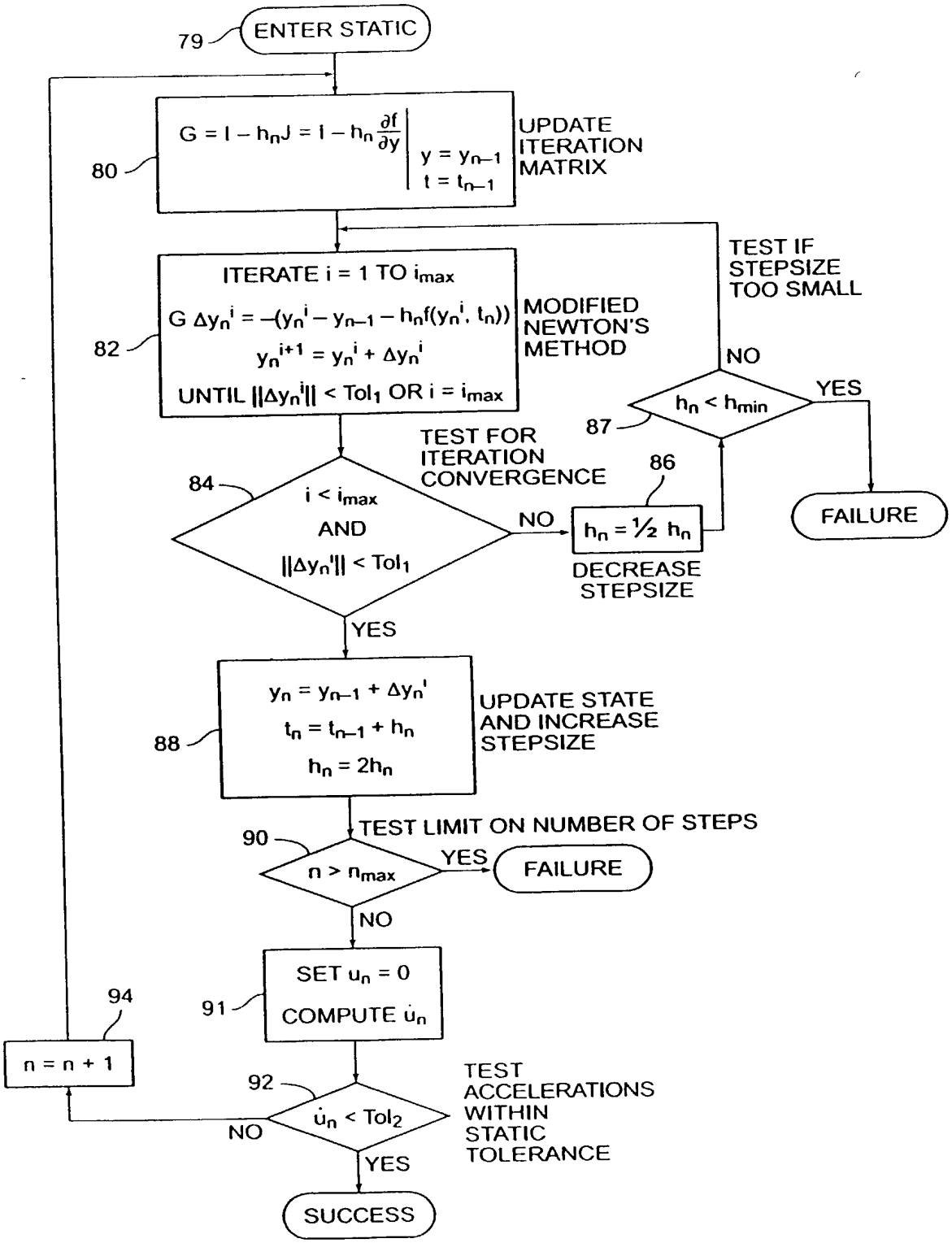
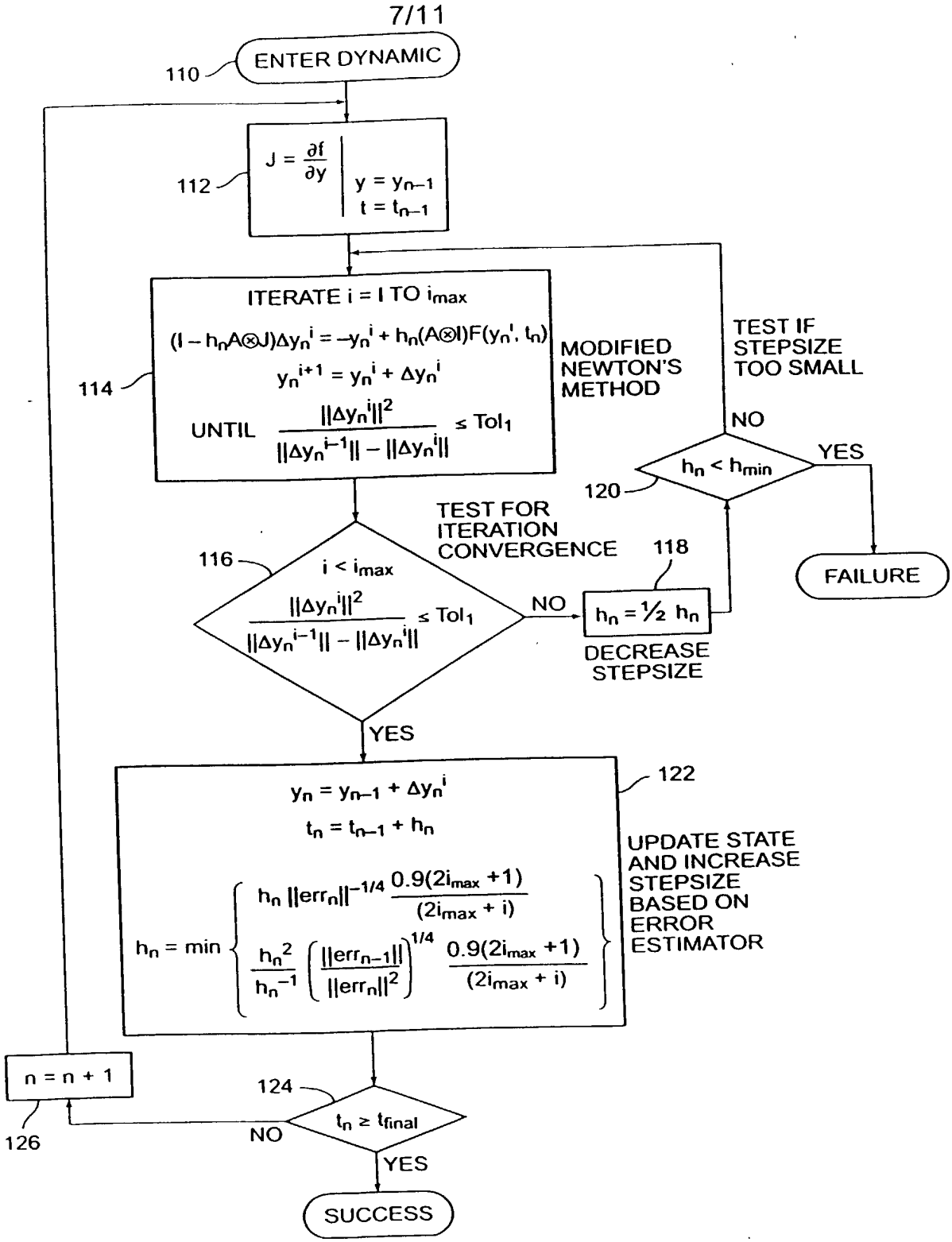

79
ENTER STATIC
80
$G = I - h_n J = I - h_n \frac{\partial f}{\partial y}\Big|_{\substack{y = y_{n-1} \\ t = t_{n-1}}}$
UPDATE ITERATION MATRIX
82
ITERATE i = 1 TO i_{max}
$G\,\Delta y_n^i = -(y_n^i - y_{n-1} - h_n f(y_n^i, t_n))$
$y_n^{i+1} = y_n^i + \Delta y_n^i$
UNTIL $\|\Delta y_n^i\| < Tol_1$ OR $i = i_{max}$
MODIFIED NEWTON'S METHOD
TEST IF STEPSIZE TOO SMALL
87
$h_n < h_{min}$
NO
YES
FAILURE
TEST FOR ITERATION CONVERGENCE
84
$i < i_{max}$ AND $\|\Delta y_n'\| < Tol_1$
NO
86
$h_n = \frac{1}{2} h_n$
DECREASE STEPSIZE
YES
88
$y_n = y_{n-1} + \Delta y_n'$
$t_n = t_{n-1} + h_n$
$h_n = 2h_n$
UPDATE STATE AND INCREASE STEPSIZE
TEST LIMIT ON NUMBER OF STEPS
90
$n > n_{max}$
YES
FAILURE
NO
91
SET $u_n = 0$
COMPUTE $\dot{u}_n$
92
$\dot{u}_n < Tol_2$
NO
YES
TEST ACCELERATIONS WITHIN STATIC TOLERANCE
94
n = n + 1
SUCCESS

FIG. 6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ENTER DYNAMIC
110
$J = \frac{\partial f}{\partial y}$ | $y = y_{n-1}$, $t = t_{n-1}$
112
ITERATE i = I TO i_{max}
$(I - h_n A \otimes J)\Delta y_n^i = -y_n^i + h_n(A \otimes I)F(y_n^i, t_n)$
$y_n^{i+1} = y_n^i + \Delta y_n^i$
UNTIL $\frac{\|\Delta y_n^i\|^2}{\|\Delta y_n^{i-1}\| - \|\Delta y_n^i\|} \le Tol_1$
114
MODIFIED NEWTON'S METHOD
TEST IF STEPSIZE TOO SMALL
NO
YES
$h_n < h_{min}$
120
FAILURE
TEST FOR ITERATION CONVERGENCE
116
$i < i_{max}$
$\frac{\|\Delta y_n^i\|^2}{\|\Delta y_n^{i-1}\| - \|\Delta y_n^i\|} \le Tol_1$
NO
$h_n = \frac{1}{2} h_n$
118
DECREASE STEPSIZE
YES
$y_n = y_{n-1} + \Delta y_n^i$
$t_n = t_{n-1} + h_n$
$h_n = \min \left\{ h_n \|err_n\|^{-1/4} \frac{0.9(2i_{max}+1)}{(2i_{max}+i)}, \frac{h_n^2}{h_n^{-1}} \left(\frac{\|err_{n-1}\|}{\|err_n\|^2} \right)^{1/4} \frac{0.9(2i_{max}+1)}{(2i_{max}+i)} \right\}$
122
UPDATE STATE AND INCREASE STEPSIZE BASED ON ERROR ESTIMATOR
n = n + 1
126
124
$t_n \ge t_{final}$
NO
YES
SUCCESS

FIG. 7

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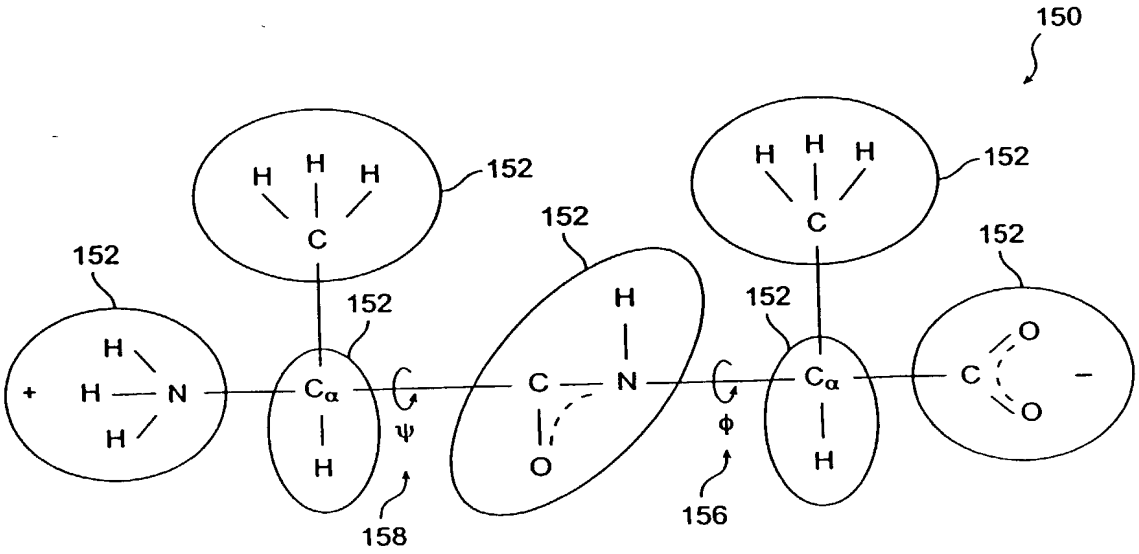

FIG. 8

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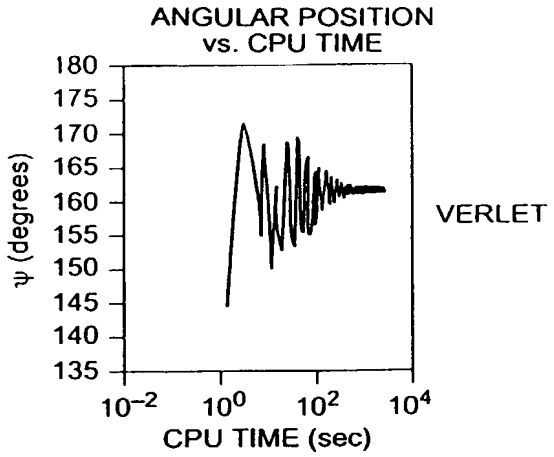

FIG. 9A

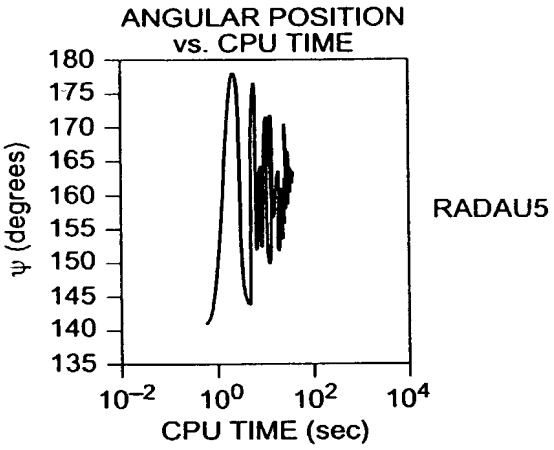

FIG. 9B

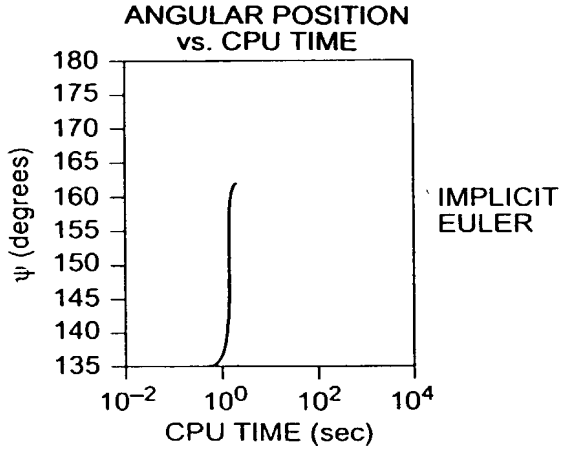

FIG. 9C

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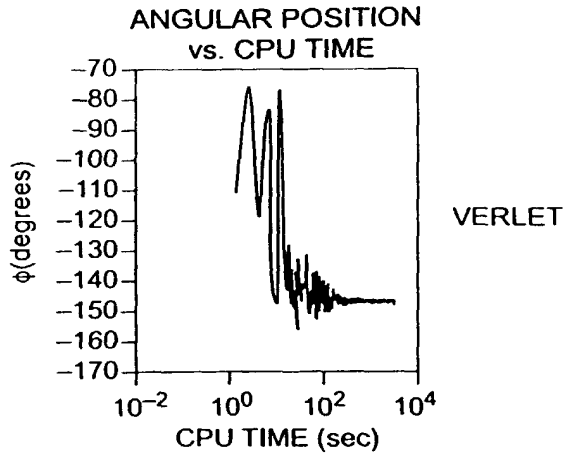

FIG. 9D

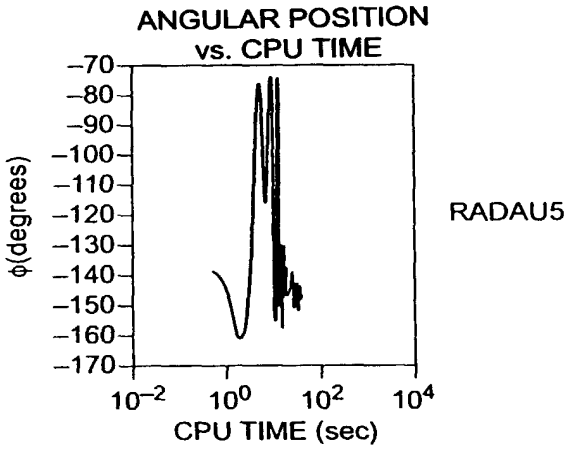

FIG. 9E

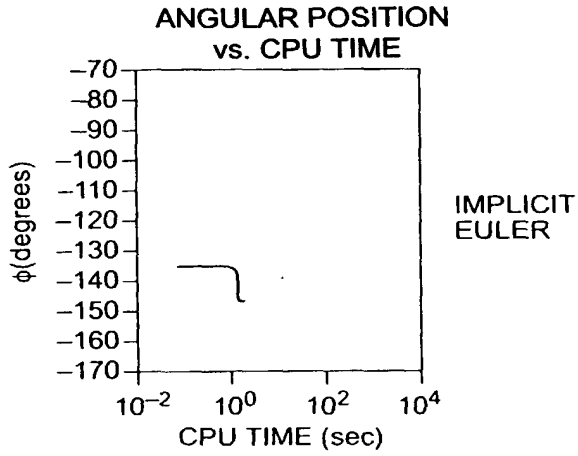

FIG. 9F

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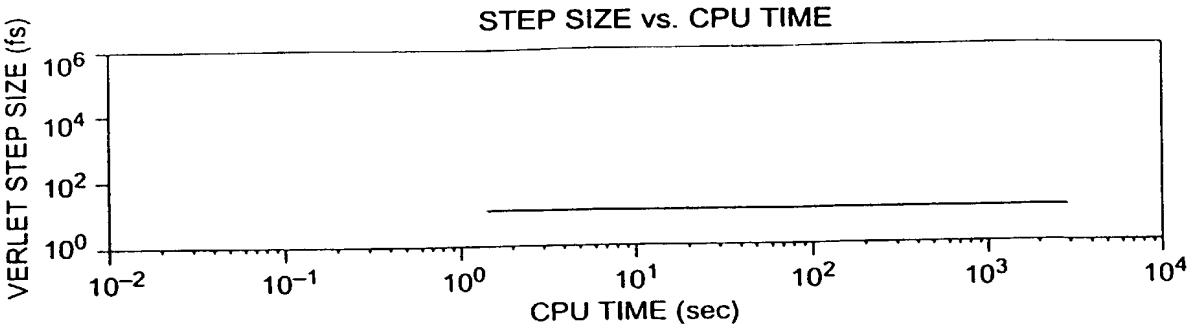

FIG. 10A

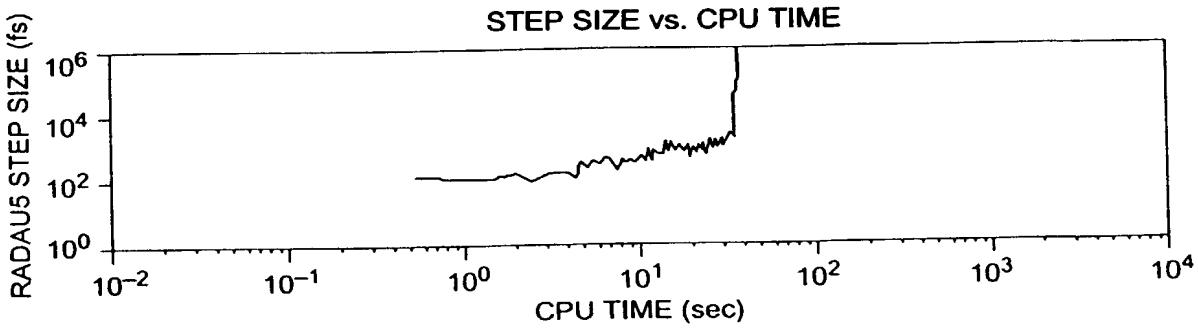

FIG. 10B

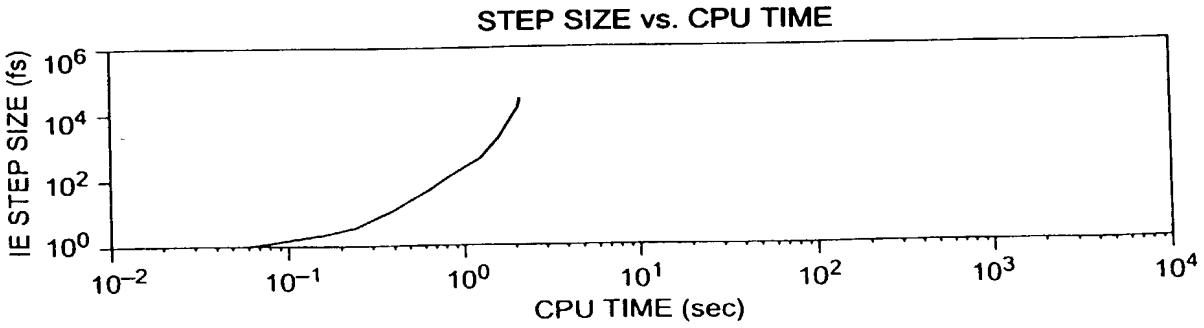

FIG. 10C